Does long-range antiferromagnetism help or inhibit superconductivity?

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We analyze the possible existence of a superconducting state in a background with long-range antiferromagnetism. We consider a generalized Hubbard model with nearest-neighbor correlated hopping in a square lattice. Near half filling, the model exhibits a *d*-wave-Bardeen-Cooper-Schrieffer (BCS) solution in the paramagnetic state. The superconducting solution would be enhanced by the antiferromagnetic background if the contribution of triplet pairs with *d*-wave symmetry and total momentum (π, π) could be neglected. However, we find that due to their contribution, the coexistence of superconductivity and long-range antiferromagnetism is ruled out for large values of the Coulomb repulsion U. Spin-density wave fluctuations (SDWF) do not change this result.

Keywords: Generalized Hubbard model, Three-body interactions, d-wave superconductor, Phase diagram, Hartree-Fock-BCS approximation

1. Introduction.

Eleven years after the discovery of the high-T_c superconductivity[1] several questions concerning the pairing mechanism and other important features of the phase-diagram of the superconducting cuprates remain without a satisfactory answer. Fortunately, there are also some aspects of the complex nature of these materials that became quite clear. It is widely accepted that the antiferromagnetic correlations play an important role in the physics of the superconducting phase and there is a good amount of evidences in favor of the d-wave symmetry of the superconducting order parameter.

The proximity between the superconducting and antiferromagnetic phases in the phase diagram of the cuprates inspired the theoreticians of this field in different ways. In some theories an antiferromagnetic background with long-range order is assumed to provide the scenario for the pairing[2–5]. In other class of theories[6–8], the pairing takes place in a background of short-range antiferromagnetic correlations with coherence lengths of only a few lattice sites. Furthermore, the different phases of the cuprates have been considered to be the result of the competition between these two different kinds of order[10]. The coexistence between antiferromagnetism and superconductivity has been discussed in other systems with conventional electron-phonon interaction[11,12] or in heavy fermion compounds[13]. In particular, some Chevrel phase compounds containing rare earths, exhibit an anomaly in the dependence of the upper critical field with temperature, as the system becomes antiferromagneticaly ordered[14]. This behavior has been explained using Eliashberg theory[12] and is due to the change in the quasiparticle-phonon interaction in the magnetically ordered phase.

The model we consider is defined by the Hamiltonian

$$\begin{aligned} H = {} & U\sum_i n_{i\uparrow}n_{i\downarrow} \; - \; \mu\sum_i (n_{i\uparrow}+n_{i\downarrow}) \\ & - \sum_{<ij>\sigma} (c^\dagger_{i\bar\sigma}c_{j\bar\sigma}+h.c)\{t_{AA}\;(1-n_{i\sigma})(1-n_{j\sigma}) \\ & + t_{BB}\; n_{i\sigma}n_{j\sigma} \\ & + t_{AB}\;[n_{i\sigma}(1-n_{j\sigma})+n_{j\sigma}(1-n_{i\sigma})]\}, \end{aligned} \tag{1}$$

where $<ij>$ denotes nearest-neighbor positions of the lattice. It was obtained from a reduction of the three-band extended Hubbard model to describe the low-energy physics of the superconducting cuprates[15,16]. The values of three different hopping integrals, t_{AA}, t_{AB}, t_{BB}, depend on the values of the parameters of the three-band Hamiltonian, i.e. on the Cu-O hopping t_{pd}, the charge-transfer energy Δ and the onsite Cu Coulomb repulsion U_d. In this paper, we consider the case $t_{AB} > t_{AA} = t_{BB}$, which corresponds to the limit $t_{pd} \ll \Delta$ and $t_{pd} \ll U_d - \Delta$. This minimal one-band model was useful to study several features of the normal state of the superconducting cuprates[15–17]. A more accurate description requires the addition of a next-nearest neighbor hopping[8,9], which we neglect here for simplicity.

Mean-field Hartree-Fock (HF) and Bardeen-Cooper-Schrieffer (BCS) approximations are the simplest approaches to the study of correlated systems. Although these techniques are not expected to be valid in the strong coupling regime ($U \to \infty$)[18] they can give valuable insight within the weak to intermediate coupling ones. In particular, the transition to the insulating spin-density-wave (SDW) phase that takes place at finite U for $t_{AB} < t_{AA} = t_{BB}$ is described with the SDW-HF approximation with acceptable quantitative precision[19,20]. We previously studied the phase diagram of (1) using BCS and SDW-HF for the same relation of hopping parameters considered here[21]. We found that the correlated-hopping term gives rise to an effective pairing interaction with components in the s- and d-wave channels. While the s-wave BCS solution is stable for low densities, the BCS solution with d-wave symmetry exists in the paramagnetic phase near half filling, within the same range of densities as the SDW-HF solution. The latter solutions are nearly degenerate at $U = 0$. However, for finite U the SDW solution is the one with the lowest energy.

The aim of this work is to investigate the possible coexistence of both kinds of order near half filling. The density of states in the split band structure of the antiferromagnetic state has a van Hove singularity at negative energies and it is further enhanced by the opening of an antiferromagnetic gap. This situation certainly enhances the magnitude of the BCS-gap within a range of densities close to that corresponding to the optimal doping of the cuprates. Such a favorable situation is the main ingredient of the first class of theories above mentioned. However, due to the broken symmetry of the antiferromagnetic state, not only singlet but also triplet pairs are coupled by the attractive interaction. We show that for certain kind of interactions, like the one considered here, or the exchange interaction $J\sum_{<ij>}\mathbf{S}_i\cdot\mathbf{S}_j$ of $t-J$-like models, both contributions have opposite sign and tend to cancel in the strong coupling limit. We also show that this tendency is not modified by spin-density wave fluctuations (SDWF) treated within the random-phase approximation (RPA). This kind of behavior might be related to the physics of the underdoped materials.

In section 2 we describe the mean-field picture and discuss the results. Section 3 contains the analysis of the RPA fluctuations. We summarize and interpret our results, and compare them with other theories in section 4.

2. Mean-field solution.

It is convenient to separate the correlated hopping terms of the Hamiltonian (1) in one- two- and three-body contributions. The complete Hamiltonian reads

$$H = U\sum_i n_{i\uparrow}n_{i\downarrow} + \sum_{<ij>\sigma}(c^\dagger_{i\bar\sigma}c_{j\bar\sigma} + h.c.)\{-t + t_2\,(n_{i\sigma}+n_{j\sigma}) + t_3\,n_{i\sigma}n_{j\sigma}\}, \tag{2}$$

where $t = t_{AA}$, $t_2 = t_{AA} - t_{AB}$ and $t_3 = 2t_{AB} - t_{AA} - t_{BB}$. Details about the mean-field decoupling of the three-body terms can be found in[19–22]. For simplicity, in what follows, we do not take into account BCS terms with s-wave symmetry. As shown in Ref.[21], these terms are relevant only for very high doping.

The effective one-body Hamiltonian can be written as:

$$\begin{aligned} H_{MF} = C &- \sum_{i\sigma}[\mu_{ef}\sigma e^{i\mathbf{Q}\cdot\mathbf{R}_i}(Um/2+4t_3\tau)]n_{i\sigma} \\ &- t_{eff}\sum_{<ij>\sigma}(c^\dagger_{i\sigma}c_{j\sigma}+h.c.) \\ &+ \sum_{i,(\delta=\mathbf{x},\mathbf{y})} b_{i\delta}(c^\dagger_{i+\delta\uparrow}c^\dagger_{i\downarrow} - c^\dagger_{i+\delta\downarrow}c^\dagger_{i\uparrow} + h.c.), \end{aligned} \tag{3}$$

where

$$\begin{aligned} \mu_{ef} &= \mu - (Un/2 + 8t_2\tau + 4t_3\tau n) \\ t_{eff} &= t - t_2 n + t_3[3\tau^2 + \varphi_{ix}^2 - (n^2 - m^2)/4] \\ b_{i\delta} &= -2t_3\tau\varphi_{i\delta} \\ C/L &= -U(n^2-m^2)/4 - 8t_2 n\tau \\ &\quad + 4t_3[4\tau(\varphi_{ix}^2+\tau^2) + m^2 - n^2]. \end{aligned} \tag{4}$$

The staggered magnetization $\langle n_{i\uparrow}\rangle - \langle n_{i\downarrow}\rangle = me^{i\mathbf{Q}\cdot\mathbf{R}_i}$, $\tau = \langle c^\dagger_{i+\delta\sigma}c_{i\sigma}\rangle$, and $\varphi_{i\delta} = \langle c^\dagger_{i+\delta\uparrow}c^\dagger_{i\downarrow}\rangle$, with $\delta = \mathbf{x},\mathbf{y}$, must be determined self-consistently. $n = n_\uparrow + n_\downarrow$ is the particle density, L is the number of sites of the lattice, $\mathbf{Q} = (\pi,\pi)$ and $\mathbf{R}_i$ denotes the atomic position. Note that $\varphi_{ix} = -\varphi_{iy}$ for the solution with d-wave symmetry.

In the paramagnetic phase $m = 0$ and the amplitude of the d-wave BCS gap φ_{ix} is independent of U[21]. The critical temperature T_c, as a function of doping is shown in Fig. 1. As within this range of densities the SDW solution ($m \neq 0$ and $\varphi_{ix} = 0$) has lower free energy that the BCS one, we consider a mean field solution with both order parameters different from 0. Due to the symmetry of the SDW background, the values of φ_{ix} depend on whether i belongs to the sublattice in which the $\uparrow$ or $\downarrow$ spins are the majority ones. The Fourier transforms of the self consistent parameters of this solution are:

$$\begin{aligned} n &= \frac{1}{L}\sum_{k\sigma}{}^{'}\,(\langle c^\dagger_{k\sigma}c_{k\sigma}\rangle + \langle c^\dagger_{k+Q\sigma}c_{k+Q\sigma}\rangle), \\ m &= \frac{2}{L}\sum_{k}{}^{'}\,\langle c^\dagger_{k\uparrow}c_{k+Q\uparrow}\rangle \\ \tau &= \frac{1}{L}\sum_{k}{}^{'}\,e^{i\mathbf{k}\cdot\delta}(\langle c^\dagger_{k\sigma}c_{k\sigma}\rangle - \langle c^\dagger_{k+Q\sigma}c_{k+Q\sigma}\rangle) \\ \varphi_{ix} &= \frac{1}{L}\sum_{k}{}^{'}\,e^{ik_x\delta_x}[(\langle c^\dagger_{k\uparrow}c^\dagger_{-k\downarrow}\rangle - \langle c^\dagger_{k+Q\uparrow}c^\dagger_{-(k+Q)\downarrow}\rangle) \\ &\quad + e^{i\mathbf{Q}\cdot\mathbf{R}_i}(\langle c^\dagger_{k+Q\uparrow}c^\dagger_{-k\downarrow}\rangle - \langle c^\dagger_{k\uparrow}c^\dagger_{-(k+Q)\downarrow}\rangle)] \\ &= \varphi^0 + e^{i\mathbf{Q}\cdot\mathbf{R}_i}\varphi^Q, \end{aligned} \tag{5}$$

where $\sum'_k$ denotes a summation over k within the reduced Brillouin zone. φ^Q is, in general, a complex quantity. There is also an imaginary term in τ, which involves mean values of the form $\langle c^\dagger_{k+Q\sigma}c_{k\sigma}\rangle$. However, all the parameters are real for the lowest-energy solution. Note that φ^Q is the mean value of the $S_z = 0$ projection of a nearest-neighbor triplet pair[10]. This is a consequence of the breaking of time-reversal symmetry in the SDW state.

As usual, the normal terms of the mean-field Hamiltonian are diagonalized by the canonical transformation:

$$\begin{aligned} c_{k\sigma} &= u_k\gamma^{(-)}_{k\sigma} - \sigma v_k\gamma^{(+)}_{k\sigma}, \\ u_k &= \sqrt{\frac{1}{2}(1+\frac{\epsilon_k}{E_k})}, \\ c_{k+Q\sigma} &= \sigma v_k\gamma^{(-)}_{k\sigma} + \sigma u_k\gamma^{(+)}_{k\sigma}, \\ v_k &= \sqrt{\frac{1}{2}(1-\frac{\epsilon_k}{E_k})}, \end{aligned} \tag{6}$$

where $\gamma^{(-)}_{k\sigma}$, $\gamma^{(+)}_{k\sigma}$ are defined on the valence and conduction bands with dispersion relations $E^\pm_k = \pm E_k$, respectively, where $E_k = \sqrt{\epsilon_k^2 + \Delta^2}$, $\epsilon_k = -2t_{ef}(\cos k_x + \cos k_y)$, and $\Delta = m(U/2 + 4t_3\tau)$. The anomalous terms are not exactly diagonalized by (6). For example

$$\begin{aligned} c^\dagger_{k\uparrow}c^\dagger_{-k\downarrow} &= u_k^2\gamma^{(-)\dagger}_{k\uparrow}\gamma^{(-)\dagger}_{-k\downarrow} - v_k^2\gamma^{(+)\dagger}_{k\uparrow}\gamma^{(+)\dagger}_{-k\downarrow} \\ &\quad + u_k v_k(\gamma^{(-)\dagger}_{k\uparrow}\gamma^{(+)\dagger}_{-k\downarrow} - \gamma^{(+)\dagger}_{k\uparrow}\gamma^{(-)\dagger}_{-k\downarrow}). \end{aligned} \tag{7}$$

Below half filling and for sufficiently large magnitude of the charge gap Δ, the interband pairs can be neglected. In the two-band basis (6) the mean-field Hamiltonian (3) results:

$$H^{MF} = \sum_{k\alpha}[\sum_\sigma(\xi^\alpha_k\gamma^{\alpha\dagger}_{k\sigma}\gamma^\alpha_{k\sigma}) - (\Delta^{\alpha s}_k\gamma^{\alpha\dagger}_{k\uparrow}\gamma^{\alpha\dagger}_{-k\downarrow} + h.c.)], \tag{8}$$

with $\alpha = +, -$, and

$$\xi_k^\alpha = E_k^\alpha - \mu_{ef},$$
$$\Delta_k^{\alpha s} = (\alpha\, \varphi^0 + 2u_k v_k \varphi^Q)\; 4t_3\tau(\cos k_x - \cos k_y). \quad (9)$$

After a Bogoliubov transformation, the set of self-consistent equations can be cast as:

$$n = 1 - \frac{1}{L}\sum_{k\alpha}{}' \; \frac{\xi_k^\alpha}{\lambda_k^\alpha}(1 - 2f(\lambda_k^\alpha)),$$

$$\tau = \frac{1}{2L}\sum_{k\alpha}{}' \; \frac{\epsilon_k \cos k_x}{E_k}\; \alpha\; \frac{\xi_k^\alpha}{\lambda_k^\alpha}(1 - 2f(\lambda_k^\alpha)),$$

$$m = m\,(\frac{U}{2} + 4t_3\tau)\; \frac{1}{2L}\sum_{k\alpha}{}' \; \frac{1}{E_k}\; \alpha\; \frac{\xi_k^\alpha}{\lambda_k^\alpha}\; (1 - 2f(\lambda_k^\alpha)),$$

$$\varphi^0 = \frac{1}{2L}\sum_{k\alpha}{}' \; \alpha\; (1 - 2f(\lambda_k^\alpha))\; \frac{\Delta_k^{\alpha s}}{\lambda_k^\alpha}\; \cos k_x,$$

$$\varphi^Q = -\frac{1}{2L}\sum_{k\alpha}{}' \; 2u_k v_k\; (1 - 2f(\lambda_k^\alpha))\; \frac{\Delta_k^{\alpha s}}{\lambda_k^\alpha}\; \cos k_x, \quad (10)$$

where $\lambda_k^\alpha = \sqrt{(\xi_k^\alpha)^2 + (\Delta_k^{\alpha s})^2}$ and $f(\lambda_k^\alpha) = 1/(1 + \exp(\beta\lambda_k^\alpha))$, with the temperature $T = 1/\beta$ in units where the Boltzmann constant $k_B = 1$. Notice that in a SDW background φ^0, φ^Q depend on U through u_k, v_k and λ_k^α. It is apparent from Eqs. (9-10) that these quantities contribute with opposite signs to the superconducting gap. At first sight it seems to be valid to neglect the contributions of the triplets φ^{Q2} to the BCS gap. Under this assumption the dependence of the mean-field critical temperature as a function of doping is shown by the solid circles in Fig. 1. The maximum of T_c occurs for values of the chemical potential μ_{ef} equal to the energy of the van Hove singularity of the density of states of the SDW solution. As this density of states is enhanced with respect to the non-interacting one, the value of the maximum T_c is, thus, enhanced with respect to the value corresponding to the paramagnetic solution for the same parameters. However, it can be easily seen from Eq. (10) that $\varphi^0 \to -\varphi^Q$ as $U \gg t$. In other words, as the staggered magnetization increases to values closer to that of the Neel state ($m = 1$), the absolute value of the contributions of triplet and singlet states become equal and the superconducting solution disappears. In the weak coupling regime, the superconducting gap does not vanish. It is, however, highly reduced with respect to that of the paramagnetic phase. For example: for optimum doping, $\varphi^0 = 0.226 \times 10^{-2}$, $\varphi^Q = -0.198 \times 10^{-2}$ for $U = 6t$, while $\varphi^0 = 0.122 \times 10^{-2}$, $\varphi^Q = -0.112 \times 10^{-2}$ for $U = 8t$. When the contribution of triplets is neglected, $\varphi^0 = 0.283 \times 10^{-1}$ for optimum doping and $U = 8t$. The maximum value of φ_x for the paramagnetic solution is $\varphi_x = 0.187 \times 10^{-1}$, independently of the magnitude of U. For $U > 8t$ we were not able to find the numerical solution of φ^0, φ^Q. One might expect that including magnetic fluctuations, the singlet contribution, and with it the superconducting order parameter is enhanced. This is discussed in the next section.

3. RPA fluctuations.

The complete treatment of the fluctuations of the antiferromagnetic background of the doped system is a quite hard task. The doping on the Neel state is expected to introduce instabilities towards the formation of incommensurate and spiral SDW kind of ordering[23] as well as quantum transitions to a quantum-disordered phase with antiferromagnetic short-range order, depending on the topology of the Fermi surface[24]. In this section, we de not consider these effects at all, and we concentrate in the study of the usual magnon SDWF, assuming that the doping does not affect the long-range order of the background. Even when this assumption is only strictly valid at half filling or for a strongly underdoped system, it is frequently used in several theories of the high-T_c, as mentioned in the introduction. For the Hubbard model at half filling, these SDWF within the RPA approximation were shown to be enough to recover the value of the local magnetization $\langle S_z \rangle$ of the Heisenberg model in the limit of $U \gg t$[3,27]. These fluctuations were further proposed to mediate the pairing interaction in the SDW background[3,25]. However, a more detailed study of the effective interactions for the Hubbard model[26,27] indicated that in fact they do not provide any pairing mechanism. In what follows, we analyze if they can correct the cancelation effect between pairs with total momentum 0 and Q presented in the previous section. In the following, we restrict our study to $T = 0$.

The three-body terms are reduced to two-body ones in this level of approximation following a similar procedure as with the Hartree-Fock decoupling[22]. It is found (up to a constant):

$$\begin{aligned} t_3 \sum_{<ij>\sigma} \quad & [\frac{n}{2}\, c_{i\sigma}^\dagger c_{j\sigma}\, (n_{i-\sigma} + n_{j-\sigma}) \\ & - \tau\, (c_{j\sigma}^\dagger c_{i\sigma} c_{j-\sigma}^\dagger c_{i-\sigma} \;+\; h.c) \\ +2 \quad & \tau\, (\, n_{i\sigma} n_{j\sigma} \;-\; c_{i\sigma}^\dagger c_{j-\sigma}^\dagger c_{i-\sigma} c_{j\sigma})]. \end{aligned} \quad (11)$$

The terms of the first line of Eq. (11) contribute only to the renormalization of the band-width and of the chemical potential, and for low-densities to the BCS-s-wave solution, but they do not couple with the SDWF. In the SDW background, the first term of the second line of Eq. (11) gives the same contribution as $4t_3\tau\ \sum_{<ij>}\ S_i^z S_j^z$

plus a nearest-neighbor repulsion, which is also reflected in the expression of the charge gap of the SDW solution. The second term, can be written as

$$2t_3\tau \sum_{<ij>} (S_i^+ S_j^- + S_i^- S_j^+), \tag{12}$$

with $S_i^+ = c_{i\uparrow}^\dagger c_{i\downarrow}$. Putting both latter contributions together, a Heisenberg interaction with antiferromagnetic coupling $J = 4t_3\tau$ is obtained. The pairing terms come from Eq. (12) and they couple with the transverse SDWF. Longitudinal SDWF do not contribute to the pairing mechanism within the present approach. Thus, we concentrate on the transverse channel. Writing Eq. (12) in the two-band SDW basis (Eq. (6)) and keeping only the terms of the valence band, which are the relevant ones for the superconductivity bellow half filling, it is found

$$\frac{1}{N} \sum_{k,q}{}' U_q \; (1 \; - \; 4u_k v_k u_{k+q} v_{k+q}) \\ \gamma_{k+q\uparrow}^{(-)\dagger} \gamma_{-(k+q)\downarrow}^{(-)\dagger} \gamma_{-k\downarrow}^{(-)} \gamma_{k\uparrow}^{(-)}, \tag{13}$$

with

$$U_q = -4t_3\tau \; (\cos q_x + \cos q_y). \tag{14}$$

While the first term contains the contributions of pairs with 0-momentum:

$$c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger c_{-(k+q)\downarrow} c_{k+q\uparrow}, \\ c_{k+Q\uparrow}^\dagger c_{-(k+Q)\downarrow}^\dagger c_{-(k+q+Q)\downarrow} c_{(k+q+Q)\uparrow}, \tag{15}$$

the second term is obtained from the contributions of pairs of triplets with momentum Q:

$$c_{k\uparrow}^\dagger c_{-(k+Q)\downarrow}^\dagger c_{-(k+q+Q)\downarrow} c_{(k+q)\uparrow}. \tag{16}$$

As discussed in the previous section, both terms tend to cancel each other.

The spin susceptibility of the SDW state is a 2×2 matrix with diagonal elements $\chi^{+-}(q,q;\omega)$, $\chi^{+-}(q+Q,q+Q;\omega)$ and off-diagonal ones $\chi^{+-}(q+Q,q;\omega)$, $\chi^{+-}(q,q+Q;\omega)$[3,25–27]. The matrix elements of the bare susceptibility with total momentum $\mathbf{Q}$ (off-diagonal matrix elements) do not contribute in the static case considered here[24]. Away from half filling, the full RPA susceptibility, has interband as well as intraband contributions. The Goldstone modes of the Neel state are obtained from the poles of the interband part of the full susceptibility. In this case from the solution of:

$$1-(U-4t_3\tau U_q)\chi_0^{+-}(q,\omega) = 0, \qquad \omega \sim 0, \qquad \mathbf{q} \sim \mathbf{Q}, \tag{17}$$

with U_q given in Eq. (14) and $\chi_0^{+-}(q,\omega)$, the diagonal matrix elements of the bare susceptibility. This equation reduces to the gap equation of the SDW mean-field solution, for $\omega = 0$, $\mathbf{q} = \mathbf{Q}$, indicating the consistency of the approach. The intraband contribution accounts for the instabilities of the SDW antiferromagnetic background with long-range order and for the transition to the quantum-disordered state[24,27] and we do not consider them in the present work. When treated within the magnon-pole approximation[3,27], the interband terms result

$$\chi^{+-}(q,q;\omega) = -\frac{1}{2}\sqrt{\frac{1-\eta_q}{1+\eta_q}}\,[\frac{1}{\omega-\Omega_q+i\delta} \\ - \frac{1}{\omega+\Omega_q-i\delta}] \\ \chi^{+-}(q,q+Q;\omega) = -\frac{1}{2}\,[\frac{1}{\omega-\Omega_q+i\delta} \\ + \frac{1}{\omega+\Omega_q-i\delta}], \tag{18}$$

with $\Omega_q = 2J_{ef}\sqrt{1-\eta_q^2}$, and $\eta_q = (\cos q_x + \cos q_y)/2$. The effective antiferromagnetic exchange coupling is defined from the dispersion relation of the spin waves. Following usual procedures[3,25,27], it is obtained for the present case $J_{ef} = 4t_{ef}^2/U + 4t_3\tau$. From Eq. (10), it can be seen that at half filling $\tau \sim \langle cosk_x\rangle/\Delta \sim 2/(\pi^2\Delta)$. Thus, in the limit $U \to \infty$, $t_{ef} \to t_{AB}$ and $J_{ef} \to 4t_{AB}^2/U$, as expected from the results of a canonical transformation on Eq. (1) for large U.

The fermion-fermion interactions constructed from the corresponding fermion-magnon ones (see Fig. 8 of Ref.[3]) are:

$$\frac{1}{N}\sum_{k,q}{}' [-\,f_1(k,q)\,V(q,q) \;+\; f_2(k,q)\,V(q+Q,q+Q) \\ +\,f_3(k,q)\,(V(q,q)-V(q+Q,q+Q))] \\ \gamma_{k+q\uparrow}^{(-)\dagger} \gamma_{-(k+q)\downarrow}^{(-)\dagger} \gamma_{-k\downarrow}^{(-)} \gamma_{k\uparrow}^{(-)}, \tag{19}$$

where

$$f_1(k,q) \;=\; u_{k+q}^2 u_k^2 + v_{k+q}^2 v_k^2, \\ f_2(k,q) \;=\; v_{k+q}^2 u_k^2 + u_{k+q}^2 v_k^2, \\ f_3(k,q) \;=\; 2\,u_{k+q} v_{k+q} u_k v_k, \\ V(q,q) = (U-U_q)^2 \chi^{+-}(q,q;\omega=0). \tag{20}$$

As in the case of the bare interaction, we kept only terms on the valence band. The first (second) line of Eq. (19) contains the contributions of pairs with total momentum 0 (Q). The bare interaction (14) has components in the

d-wave- as well as in the s-wave-channel. The relevant terms for the d-wave part, are those with $\mathbf{k}$ near $(0,\pi)$ and $\mathbf{q}$ near $(0,0)$ as well as symmetry-related points. SDWF would help to superconductivity in the case that the second line of Eq. (19) tends to cancel the second term of Eq. (13) while the first line of Eq. (19) vanishes or has the same sign as the first term of Eq. (13) for these wave vectors. For $\Delta \gg t$, $E_k \sim \Delta$ and $f_3(k,q) \to 1/2$. Expanding the structure factors $f_1(k,q)$, $f_2(k,q)$, the first line of Eq. (19) can be written as

$$-\frac{1}{2}\left(V(q,q) - V(q+Q,q+Q)\right) - \frac{\epsilon_k \epsilon_{k+q}}{\Delta^2}\left(V(q,q) + V(q+Q,q+Q)\right). \tag{21}$$

The first term of Eq. (21) exactly cancels the second line of Eq. (19). The remaining term, which comes from pairs with momentum 0, can be expanded for small $\mathbf{q}$,

$$\begin{aligned} V(q,q) + V(q+Q,q+Q) \sim \frac{2}{J_{ef}} \, [\, & \frac{(U+8t_3\tau)^2}{q_x^2+q_y^2} \\ & - 8t_3\tau(4t_3\tau + U) \,] \\ \frac{\epsilon_k \epsilon_{k'}}{\Delta^2} \sim \frac{(\mathbf{v_k}\cdot\delta\mathbf{k})^2}{\Delta^2}, & \end{aligned} \tag{22}$$

where $v_k^i = \partial \epsilon_k / \partial k_i|_{\mathbf{k}_0}$ and $\delta\mathbf{k} \sim \delta\mathbf{k}' = \mathbf{k} - \mathbf{k}_0 \sim \mathbf{q}$. The latter quantity is vanishingly small except for $\mathbf{k}_0 \sim (\pi/2,\pi/2)$, in which case[26,27], the effective interaction in real space is a local repulsion in the triplet-channel plus a long-range dipolar interaction and it is expected to induce spiral distortions in the antiferromagnetic state[23].

Thus, SDWF of the Neel state treated in the RPA approximation, do not modify the picture obtained at the mean-field level.

4. Conclusions and discussion.

Our results can be summarized as follows. We studied an effective one-band model for the superconducting cuprates in the underdoped regime. The model has an effective pairing interaction and a BCS- mean-field solution with d-wave symmetry in the range of doping $0 < \delta < .5$, which might be relevant for the pairing mechanism of the cuprates. However, in the mean-field level, this solution has always higher energy than the antiferromagnetic SDW one. For the case of the $t-J$ model, for which the results of strong-coupling mean-field[28] as well as numerical techniques[29], indicate that it exhibits superconductivity, the instability of the Neel state is found also at very high doping within some mean field approaches[30]. In other more phenomenological approaches, antiferromagnetic long-range order has been used to simulate the short range antiferromagnetic correlations[4,9]. In this work we explored the possibility of coexistence of both kinds of order: antiferromagnetism and superconductivity. We found that neglecting the contribution of triplet-pairs with momentum Q as done in other approaches for simplicity[2], there is an enhancement of the d-wave superconducting solution due to the modified density of states of the antiferromagnetic state with long-range order. We found, however, that both contributions are equally important and tend to cancel each other. For large values of the Coulomb repulsion U there is no chance for superconductivity and for low to intermediate values the magnitude of the superconducting gap is much weaker than that of the paramagnetic BCS solution.

Our results are more transparent when analyzed in real space. The terms of the Hamiltonian here considered, that cause the pairing, are the three-body ones. Treating them in mean-field and reducing them to two-body ones, a nearest-neighbor spin-flip antiferromagnetic interaction is found. This kind of interaction is expected to generate an effective attraction for nearest-neighbor spins in the singlet channel. In fact, in the strong-coupling limit, resonating valence bond (RVB) singlets, which are widely accepted to build up a superconducting state, are mainly a consequence of the same kind of interaction[6,8]. The formation of singlet pairs is, however, very unlikely in an antiferromagnetic background with long-range order. Spin fluctuations of the Neel state in the RPA level (interband fluctuations) do not correct this effect. For higher doping, intraband fluctuations are important and the antiferromagnetic correlations are short-range like in real materials[24]. This scenario is better described by a nearly antiferromagnetic Fermi liquid picture[7]. We expect the pairing mechanism contained in this model to be active within such a background. This is confirmed by preliminary results[31].

In other theories, like the antiferromagnetic van Hove mechanism[4,9] or the spin-polaron model[5], the superconductivity is mainly determined by kinetic reasons. These theories assume that holes like to propagate in the long-range antiferromagnetic background distorting it as less as possible. In the first case, holes are assumed to move within the same sublattice and to experience an attractive interaction $\sim -0.6J = J\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$ between nearest-neighbor holes. Note however, that the results of the previous section and previous works[27] suggest that it is not valid to replace the exchange interaction by a nearest-neighbor attraction in the Neel state. Numerical calculations also show that the antiferromagnetic van Hove scenario does not represent correctly the physics of realistic $t-J$-like models[32]. The $t-J$ model contains, however, an explicit nearest-neighbor attraction of magnitude $J/4$, which plays a relevant role in most of the

strong-coupling approaches[6,8,28,29]. In the case of the spin-polaron model[5], this nearest-neighbor attraction is neglected and hopping of a hole between both sublattices is allowed by the occurrence of a local spin-flip in the slave-fermion representation used. The holes become paired through the hole-magnon interaction originated in the hopping process and the resulting T_c in this strong-coupling approach becomes appreciable in contrast to our weak coupling results and those of Ref.[27]. It is quite easy to inspect the correlated hopping terms and observe that in the present model no terms like $c^{\dagger}_{j\uparrow}c_{i\uparrow}S^{+}_{i}$ are generated within the mean-field treatment. Such terms could lead to a polaron-like picture in the weak-coupling formalism.

A BCS mean-field approximation does not lead to superconductivity in the ordinary Hubbard model ($t_{ab} = t$) with $U > 0$. There are instead, several calculations of the superconducting gap with other mean-field Eliashberg-like theories, based on the fluctuation-exchange approximation (FLEX)[33], which suggest d-wave superconductivity in the model. However many numerical attempts to find evidences of superconductivity in the pure Hubbard model have been negative[34]. There are two features of the results based on the FLEX approximation that could lead one to speculate about some connection between these treatments for the Hubbard model and the results we presented here: a) within the FLEX approximation, pairing is caused by an effective attraction in the d-wave channel, which is originated by spin fluctuations in the paramagnetic phase. In the present case, pairing is originated by the interaction (12), which is precisely the nearest-neighbors static version of an effective attraction mediated by the transverse spin fluctuations. Thus, within the paramagnetic phase, superconductivity in the present model could have a similar origin as that of FLEX for the pure Hubbard model. b) As discussed in detail in Ref.[35], the FLEX approximation offers a quite poor treatment of antiferromagnetic correlations. In particular, the antiferromagnetic state is not recovered, even at half filling. The behavior of the superconducting gap within the FLEX approximation[33] is very similar to that shown in Fig. 1 for the BCS d-wave solution for $t_{AB} \neq 0$ in the paramagnetic phase. Questions arise about what could occur in the pure Hubbard model, in the case that the tendency towards long-range antiferromagnetism could be also included in some FLEX-like scheme. In connection with this latter point, it could be stressed that the effective interactions generated by the SDWF of the antiferromagnetic state of the Hubbard model[3,25–27], where shown not to be able to provide any effective attractive interaction in the d-wave channel[26,27].

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FIGURE CAPTIONS

Fig. 1. Mean-field critical temperature as a function of doping $x = 1 - n$ for $t_{AA} = t_{BB} = t$ and $t_{AB} = 1.5t$. Open circles correspond to the usual paramagnetic d-wave BCS solution. Solid circles correspond to the d-wave BCS solution in the SDW background for $U = 8t$, neglecting the contributions of triplets with total momentum $\mathbf{Q} = (\pi, \pi)$.

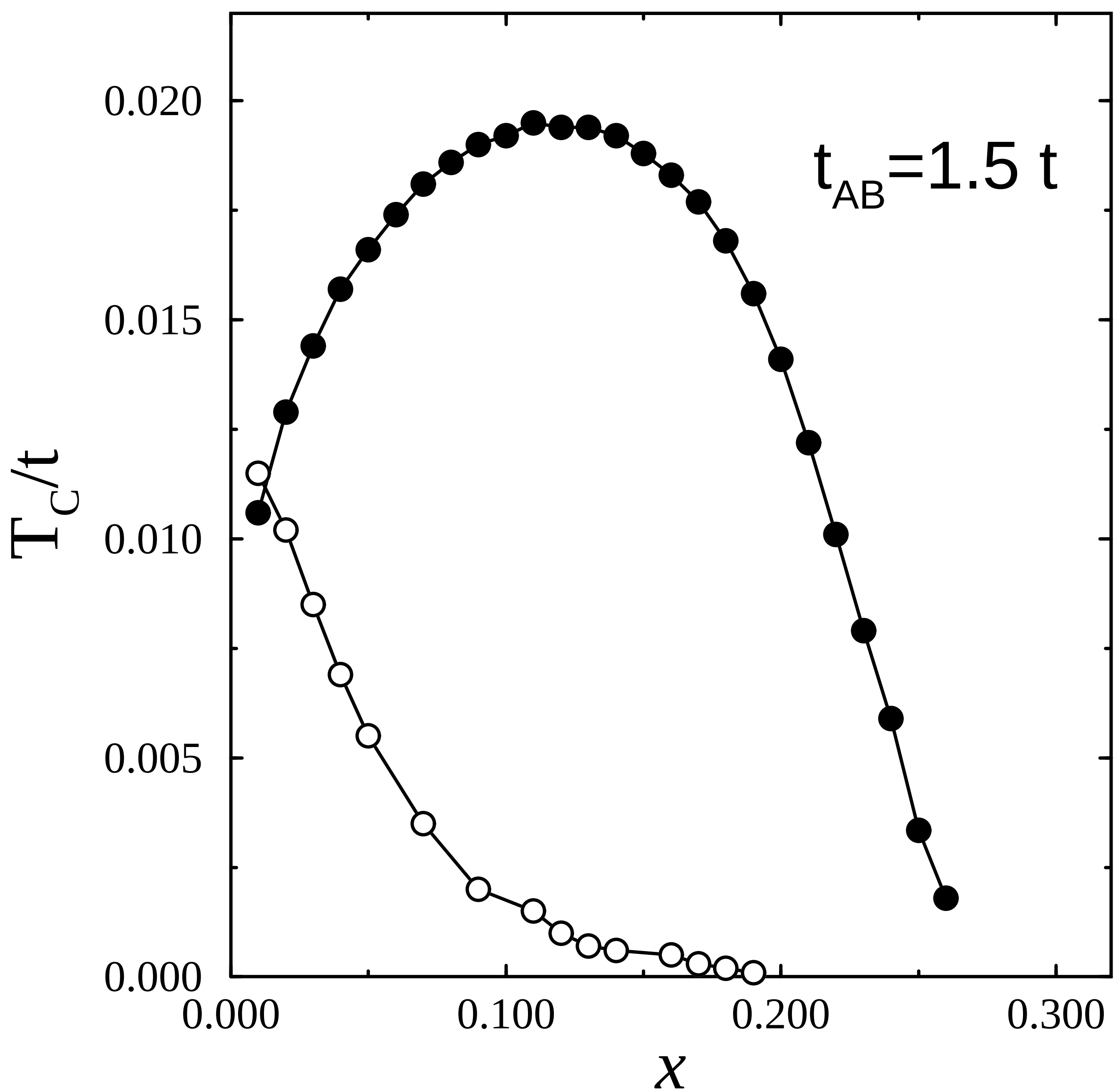

FIGURE 1